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Transient Tracers as a Problem in Control Theory

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The problem of interpreting transient tracer surveys in the ocean is formally identified as corresponding to placing a "terminal constraint" on a "distributed system boundary control problem." The mathematics available in control theory can then be brought to bear on the tracer data. Some of control theory is reviewed in the context of a simple tracer example to isolate the major issues. To use a transient tracer to invert for flow and mixing rates involves a two-step process: start with an initial model, found independently, and determine if acceptable boundary conditions drive the model to reproduce the interior transient tracer at the observation times. If the model succeeds in that reproduction, one stops; the model is adequate and need not be changed. Only if this test fails does one obtain constraints on the fluid flow and mixing, which can be invoked in parameter estimation techniques of control theory. Terminal constraint observations can also be used to estimate the tracer concentrations at earlier times using a smoothing filter.

1. INTRODUCTION

Direct inference of ocean circulation parameters (flow and mixing rates) from measurements of transient "dyes" in the ocean is not entirely straightforward. In two previous papers [*Wunsch*, 1987, 1988] (hereafter referred to P1 and P2, respectively) I began what was intended to be an exploration of procedures for making direct inferences about the circulation while simultaneously evaluating the information content of the tracer fields relative to that of more conventional oceanographic measurements.

P1 pointed out that unlike the problem of steady tracers, one had to distinguish between three distinct types of mathematical system: (1) the forward problem, (2) the inverse problem, (3) the regularization problem. The results can be summarized by recognizing that most discussions of the solution of partial differential equations focus upon the conventional, well-posed forward problem, in which perfect (in the Cauchy-Hadamard sense) boundary conditions are used to step a system forward in time and space. Almost all ocean models are formulated in this sense. Unfortunately, the problem of using oceanic observations with models (not just tracer models) is fundamentally that of making inferences about ill-posed systems. (The terminology "ill-posed" is somewhat unfortunate, suggesting shortcomings in the investigator who works with such systems. But well-posed problems exist mainly in textbooks and rarely in the universe of scientists trying to compare models with data).

The inverse problem for tracers, steady or otherwise, is easily stated: given a set of observations of a tracer $C(\mathbf{x}_i, t_i)$ distributed irregularly and with specifiable noise statistics over an interior domain and on the boundaries, infer the fluid flow parameters. For steady ocean tracers, a decade of work has led to a variety of procedures for making inferences, either in a statistical sense (e.g., maximum likelihood) or in a bounding envelope sense (see for example, *Wunsch* [1984] or *Schlitzer* [1987]).

In P1 and P2, it was shown, however, that once time is admitted to the problem in the shape of a tracer transient (while still keeping the flow field steady), inferences about the flow parameters had to be deferred until the regularization problem was solved. By regularization is meant the problem of determining whether the boundary conditions governing the evolution of the tracer field could be determined from interior, noisy observations. As is discussed in P1, regularization is equivalent to solving a diffuse system upstream and backwards in time. That such solutions are possible was demonstrated by one-dimensional pipe flow models through what is called a "whole-domain method," in which the unstable components of the solution are controlled in a global sense by treating all of space and time simultaneously. Although not an inverse problem, the methods employed are similar to those used for inverse ones.

In P2, application was made to determining ventilation rates of the eastern Atlantic thermocline, combining geostrophic and vorticity constraints with those of helium-3 (^{3}He) and tritium (^{3}H) in a three-dimensional, time-dependent system. Regularization was accomplished by writing the missing boundary conditions as unknown coefficients of a boundary Green's function. The procedures used in both papers were all variants of whole domain ones derived from inverse methods.

The great advantages of whole domain methods are their simplicity of concept, their power, and flexibility. Their great disadvantage is the rapid escalation of the computational load that occurs in three space dimensions and time. Much of the discussion in P2 concerned means to reduce the system size to one more consistent with the available data.

At the time of completion of P1, it had already become clear to me that many of the methods being employed could be unified under the general umbrella of "control theory." The purpose of this present note is to point out the formal similarity between many control problems and solutions and those involved in understanding and using ocean tracers. The calculations are freed of the many regional oceanographic problems of P2 so as to isolate the mathematical issues, which are very general. This paper is not a review of control theory; that subject is very large, subsuming major parts of modern engineering and pure and applied mathematics. Indeed, one of the obstacles to learning control methods is the overwhelming size of the literature.

2. FORMULATION

Every practical tracer situation is different and no brief discussion can possibly be all inclusive. So for purposes of illus-

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tration, the problem will be formulated as almost a "cartoon" tracer problem, abstracted from the situation in P2, as follows.

A tracer, denoted C, is supposed to satisfy a generic advection-diffusion equation of form

$$\frac{\partial C}{\partial t} + \mathbf{v} \cdot \nabla C = \nabla \alpha \nabla C - \lambda C + Q \tag{1}$$

where α is a mixing tensor, λ represents a decay rate, and Q represents interior sources and sinks.

We suppose that as with Freons, ^{3}H, and ^{3}He, a time history of the surface concentration $C(x, y, z = 0, t)$ is known, with an error $\varepsilon(\mathbf{x}, t)$ of specified mean square. Suppose further, that at time t_f, an oceanographer arrives on the scene and surveys the tracer concentration within some interior volume of ocean, obtaining a set of concentrations

$$C_d(\mathbf{x}_i, t_f) = C(\mathbf{x}_i, t_f) + \varepsilon(\mathbf{x}_i, t_f) \tag{2}$$

where ε again represents the errors (analytical and sampling). The survey time is supposed sufficiently short that we can regard all the observations as having occurred at the single time t_f.

Suppose at $t = 0$, the initial tracer distribution in the region is known $C(\mathbf{x}, t = 0) = C_0(\mathbf{x})$. C_0 may well be zero, with little or no uncertainty, as with the tracers already mentioned, if $t = 0$ is in the early 1950s (say), or it might be the result of a previous survey some years before, in which case its errors must also be accounted for.

Conventionally, data like those described (e.g., the Transient Tracers survey of the North Atlantic) have been used as follows: one takes a dynamical model (as *Sarmiento* [1983] took the K. Bryan model), imposes the boundary conditions at the surface, and computes the model distribution of tracer through time, stopping the calculation of model time t_f. The calculated tracer is compared with the measured one, and the result is deemed acceptable or not. If the results are sufficiently similar, one concludes that the tracer distribution has thus "verified" the model.

Consider now the more common problem when there are discrepancies too large to ignore. It is often asserted that the great power of tracers lies in their integration of the circulation over long distances and times. But this integration is simultaneously their great weakness. Suppose the model alluded to were "perfect," having correct flows and mixing. However, if there are slight systematic errors in the surface boundary conditions (e.g., that the tritium concentration in some region is estimated to be 10% higher than it really was for 10 years), then this small systematic error will accumulate in the model, in some cases at regions far from the initial difficulty. The final comparison between computation and measurement may well be a poor one, leading perhaps to the incorrect conclusion that the model was in error. It was this specific concern about boundary conditions which motivated P1. P2 showed that uncertainty about the tracer time history at the boundaries leads to treating the boundary conditions as part of the problem unknowns, rather than, as one is taught and teaches, as "given." The necessity of treating boundary conditions as part of the system unknowns is what leads us to control procedures.

Consider a bounded volume of ocean. Equation (1) is now supposed to govern a region with $\mathbf{v}$, α known perfectly and completely. Equation (1) can be rewritten as

$$\frac{\partial C(\mathbf{x}, t)}{\partial t} = A_1(C(\mathbf{x}, t), Q) \tag{3}$$

or, in finite differences, or finite elements, etc., as

$$\mathbf{C}(t + 1) = \mathbf{A}\mathbf{C}(t) + \mathbf{B}\mathbf{u}(t) \tag{4}$$

where the matrices $\mathbf{A}$ and $\mathbf{B}$ are constant with time (to keep the discussion as simple as possible; this assumption is not necessary). The elements of the vector $\mathbf{C}(t)$ are the values $C(\mathbf{x}_i, t)$ at the grid points $\mathbf{x}_i$ or the finite element coefficients at time t or any other proper representation of the "state" variables C. To generate simple examples, I will use an elementary 4×4 box model (Figure 1), a reduced version of that used in P2. Let the net flux of mass from box i to box j be written J_{ij}, with the resulting tracer flux, then $C_i J_{ij}$. The model is thus represented by a crude form of upstream differencing, but I emphasize that much more complex discrete representations of (1) can be written in the form (4) and the simplification to a box model does not remove any of the fundamental mathematical issues; the appendix makes this assertion explicit. The model in Figure 1 is intended to be abstract and generic to focus on the essential mathematical issues. For convenience of reference, the boxes numbered 1–4 sometimes will be referred to as the "surface" layer, which might correspond to the ocean surface layer, with the horizontal coordinate being either latitude or longitude. Explicit geographical identification is, however, neither necessary nor intended here. Similarly, the physical interpretation of the J_{ij} need not distract us; readers who wish to pursue the question are referred to P2 or *Keeling and Bolin* [1967].

Under these circumstances, for any interior box i, in the absence of sources or sinks, the time evolution is described as

$$C_i(t + 1) = C_i(t) - \lambda \Delta t C_i(t) - \frac{\Delta t}{V} \sum_j C_i(t) J_{ij} + \frac{\Delta t}{V} \sum_j C_j(t) J_{ji}$$

where the summation on j is over all neighbors to box i, Δt is the time step, and V is the box "volume." We took $\Delta t / V = 0.1$. The rows of $\mathbf{A}$ appearing in (4) sum to $1 - \lambda$, because mass conservation requires the J_{ij} and J_{ji} entering and leaving a box to sum to zero, except in the boundary boxes; λ has been set to zero here.

The term $\mathbf{Bu}$ represents the boundary conditions in the shaded boxes of Figure 1; they are being taken here as specified values of the time derivatives of the concentrations there. Unless otherwise specified, all vectors are column vectors. More generally, this term can also represent any interior sources or sinks. The separation of the structures of $\mathbf{B}$ and $\mathbf{u}$ is somewhat arbitrary; they can be chosen at the investigator's convenience. Here I have opted to let $\mathbf{B}$ consist of a matrix which specifies, through its nonzero elements, those boxes in which boundary conditions affect the interior and put interior Q, including λ, to zero. The vector $\mathbf{u}$ is chosen to be a scalar function of time producing time histories in the active boxes which are identical. To be as explicit as possible, the full $\mathbf{A}$ matrix and $\mathbf{B}$ are written out in Figure 2.

2.1. *The Forward Problem*

The forward problem is specify $\mathbf{Bu}$ (see Figure 3*a*) and calculate forward in time from an initial concentration $\mathbf{C}(t = 0) = 0$. After $t_f = 14$ time steps (define $\Delta t = 1$), the distribution of tracer in the boxes is as shown in Figure 3*b*. (P2 discusses the size of the time step necessary for stability.) For illustration, this solution is deemed the reference case: the fluxes J_{ij} are assumed to be correct, and the tracer distribution, at the end of t_f time steps is taken as "truth." Here $\mathbf{u}$ was the scalar $u = \exp(t)$, $t = 0$ to 6, $u = 0$, thereafter so that

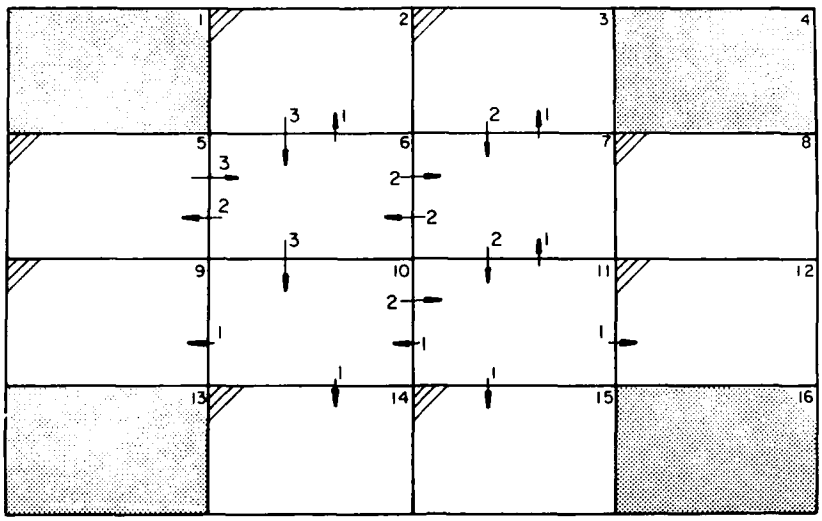

Fig. 1. Simple box model used to illustrate control form of transient tracer problem. The four corner boxes (stippled) are not involved in the calculation; boxes with partial shading are regions in which formal boundary conditions are required. The flow fields J_{ij} used in the computations are displayed with the numerical values attached. Concentrations in boundary boxes from which there is no flow into the interior are physically irrelevant ("unobservable"), e.g., box 9. Concentrations in boxes 8, 12, 14, and 15 are specified as zero. Active interior boxes are 6, 7, 10, and 11.

all boundary boxes at the top and left have the same history. B vanishes in the bottom and right boxes, fixing zero concentration there (Figure 2 (bottom)).

A simple illustration of the bias problem is obtained by recomputing in the forward direction with the boundary concentration time rate of change in box 5 artificially raised by 0.5 tracer units. At $t_f = 14$, the biased forward calculation gives the values displayed in Figure 4. The error in $\mathbf{C}(t_f)$ is caused solely by the error in the boundary conditions. (Use of the concentration time rate of change for the boundary conditions, rather than concentration itself, does exaggerate the effect of the systematic error. But the present system is being computed for only 14 time steps and basin scale models integrated for thousands of time steps would accumulate potentially massive systematic errors from concentration boundary conditions.)

2.2. *The Inverse Problem*

The oceanographer arrives with his ship at time $t = t_f$ and measures with some error the concentration shown in the boxes of Figure 3*b*, including the boundary boxes. He may also know the boundary concentrations of Figure 3*a* through time in the surface boxes, again with an error. The inverse problem is infer the J_{ij} (or, equivalently, the elements A_{ij} of equation (4)).

As is discussed in P2, unlike the steady problem this inverse calculation is nearly intractable: from one survey at $t = t_f$ we do not know $\mathbf{C}(t+1) - \mathbf{C}(t)$ on the time scale required for numerical stability in (4), and we do not know the time histories in the left boundary boxes of Figure 2.

Use of the values of $\mathbf{C}(t_f)$ to constrain the J_{ij} to make improved estimates of them by inversion must therefore be deferred, pending the outcome of the calculations described in the next section.

2.3. *The Control Problem*

Let us restate the problem. Given the $\mathbf{C}_0$, the "terminal constraint" $\mathbf{C}(t_f) = \mathbf{C}_d$, the evolution equation (4), and any restrictions we might wish to place on $\mathbf{Bu}$, determine if there exist any values of $\mathbf{u}$, such that the system (4) is carried from its initial conditions to the terminal conditions as observed. If such a $\mathbf{u}$ exists and it is acceptable, then the flow field is consistent with the transient tracer distributions. If no such $\mathbf{u}$ can be found, then the flow field is not consistent with the transient tracers, can be rejected, and hence modified. But we do not need to grapple with the problem of determining a modified flow field until it has been demonstrated that the old one is inconsistent with the observations.

An "acceptable" set of boundary conditions would be those not in conflict with what is known a priori about them. At one level, the boundary concentrations may only have to be positive to be acceptable. Or, one may have some measurements of them to which the calculations most conform within the error estimate. We will show below how to explicitly accommodate numerical values of boundary data where they are availiable. For the moment, however, attention is confined to the case where they are only required to be physically realizable (i.e., positive and not infinite in value).

It is possible to attempt simultaneously to modify the model and the boundary conditions-initial conditions, but given the size and complexity of time evolving systems, there is real advantage to being able to adopt a stepwise approach. One first asks the simpler question of whether all discrepancies can be eliminated acceptably through modification of estimates of boundary data, before setting out on the potentially long road of simultaneously modifying the model too.

The tracer survey represents a terminal constraint. It is the point to which a complex system must evolve at a given time. An analogy is the control problem of a robotic arm. At $t = 0$, a robot arm is at a known initial position, A. At $t = t_f$ it is required that the arm be in a position, B, within some tolerance, for grasping an object within some tolerance. Merely observing that the arm was initially at A at $t = 0$ and at B at t_f does not tell us the trajectory or velocity that the arm had in between. Conventional control problems are to find a trajectory from A to B that minimizes the energy required to move the arm or gives the smoothest trajectory, etc. The tracer problem consists instead of determining whether any

A =

1.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	1.00	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1.00	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	1.00	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1.00	0	0	0	0	0	0	0	0	0	0	0
0	0.30	0	0	0.30	0.20	0.20	0	0	0	0	0	0	0	0	0
0	0	0.20	0	0	0.20	0.50	0	0	0	0.10	0	0	0	0	0
0	0	0	0	0	0	0	1.00	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	1.00	0	0	0	0	0	0	0
0	0	0	0	0	0.30	0	0	0	0.60	0.10	0	0	0	0	0
0	0	0	0	0	0	0.20	0	0	0.20	0.60	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	1.00	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1.00	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	1.00	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.00

$\mathbf{B}^T$ =

0	1.00	1.00	0	1.00	0	0	0	0	0	0	0	0	0	0	0

Bu =

0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0.13	0.25	0.35	0.44	0.51	0.58	0	0	0	0	0	0	0
0	0.13	0.25	0.35	0.44	0.51	0.58	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0.13	0.25	0.35	0.44	0.51	0.58	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0

Fig. 2. (Top) **A** matrix from flow in Figure 1. (Bottom) $\mathbf{B}^T$ (**B** is here a simple time-independent column vector), providing the information on which boxes are boundary ones. There is 1 in each of the top and left boundary boxes, but corner boxes and box 9 are wholly passive as far as interior is concerned. **Bu** provides a complete time history of the driving for the reference case. In special case treated here **u** is a scalar $u(t)$. The simple form taken for **B** and **u** forces the time history in each box to be identical. Very much more complex boundary conditions can be imposed by letting **B** be a $16 \times M$ time-dependent matrix (16 is the total number of boxes), and **u** an $M \times 1$ time-dependent vector, where M is arbitrarily large.

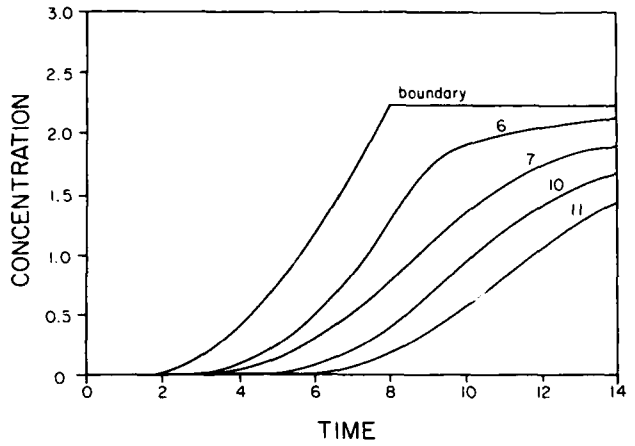

Fig. 3*a*. Concentration time histories for a 14 time step forward integration. Boundary boxes were driven by the concentration rates of change shown in Figure 2 resulting in the concentrations marked "boundary." Time histories for interior boxes are also depicted as calculated from (4).

physically acceptable trajectory exists given that the arm was observed to have been at A at $t = 0$ and at B at $t = t_f$.

The problem is mathematically interesting because the tracer "control" is represented by the boundary conditions, and they must be determined. Because the tracer system is governed by a partial differential equation, the problem is that of "distributed system boundary control." Readers interested in the general mathematical issues are referred to *Lions* [1971] or *Stavroulakis* [1983*a*, *b*].

As the intention is illustrative here, we will proceed to a specific example. Mimicking our hypothetical oceanographic case, we seek boundary histories $\mathbf{u}$ such that we minimize the objective function

$$J = [\mathbf{C}(t_f) - \mathbf{C}_d]^T \mathbf{G} [\mathbf{C}(t_f) - \mathbf{C}_d] + \sum_t \mathbf{u}^T(t)\mathbf{u}(t) \qquad (5)$$

The matrix $\mathbf{G}$ is proportional to the reciprocal covariance of the error in the terminal state observations $\mathbf{C}_d$ (equation (2)). For present purposes, it suffices to notice that by varying $\mathbf{G}$, we can weight the demand for reproduction of the terminal state survey against the demand for a minimum "energy" $\mathbf{u}$. Equation (5) is chosen as only one example of the general class of L_2 norm objective functions. We are omitting the possibility that any of the elements of the terminal state should be reproduced exactly, i.e., we do not demand that

$$C_i(t_f) = C_{di} \qquad \text{for any } i \qquad (6)$$

without error. Although the control formalism admits of such requirements (see the discussion in the work by *Luenberger* [1979]), they needlessly complicate the mathematics and are unlikely ever to be realistic in any case. The terminal state can be pushed arbitrarily close to the observations by use of $\mathbf{G}$, without encountering the degeneracy involved in imposing (6). (The fundamental difficulty is that exact satisfaction of the terminal state often renders the second term of J irrelevant, there being only one, or even no, possible values of $\mathbf{u}$ producing a fixed terminal state.)

The second term on the right of (5) is only an example, which is most appropriate if there was reason to seek the smallest mean square injection consistent with the system and the terminal constraint observations. No implication that this is necessarily the most useful such objective function is intended, and much more complex ones can be used. In section 2.4. we will extend (5) to minimize the mean square deviation from an a priori estimate which differs from the zero a priori value implicit there.

Solution of this unorthodox problem is usually obtained through either the so-called Pontryagin minimum principle, or dynamic programming methods. For systems of the present type, the minimum principle appears to be computationally more feasible. I will not derive the discrete time optimality theorem (see *Luenberger* [1979], who however refers to it as the "maximum principle" having introduced a sign change). The reader is willing, I hope, to take the theorem on faith. *Thacker and Long* [1988] derive a version of it. It can be stated fairly concisely, although not in its most general form as follows. Let H be a Hamiltonian defined as

$$H(\mathbf{C}(t), \lambda(t), \mathbf{u}(t)) = \lambda^T(t)[\mathbf{A}\mathbf{C}(t) + \mathbf{B}\mathbf{u}(t)] + \mathbf{u}^T(t)\mathbf{u}(t) \qquad (7)$$

Let the system satisfy the evolution equation (4), subject to the initial conditions $\mathbf{C}(t = 0) = \mathbf{C}_0$, and the minimum of (5) is

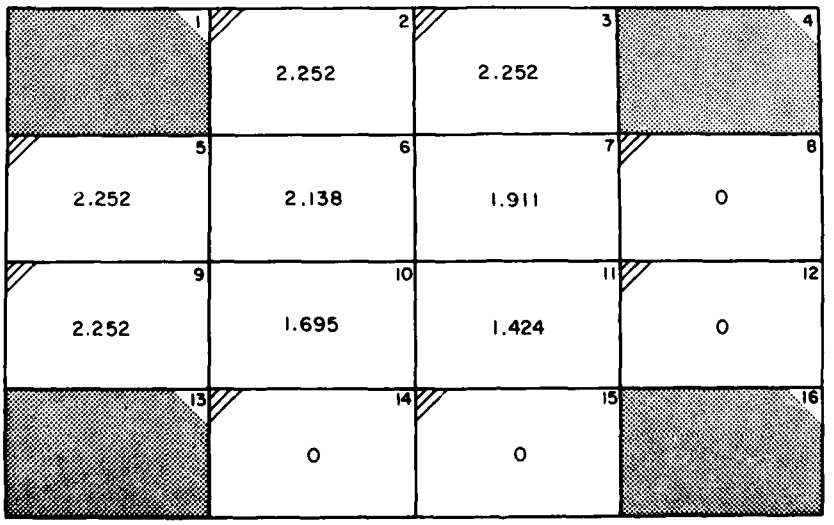

Fig. 3*b*. Concentrations at terminal time $t_f = 14$.

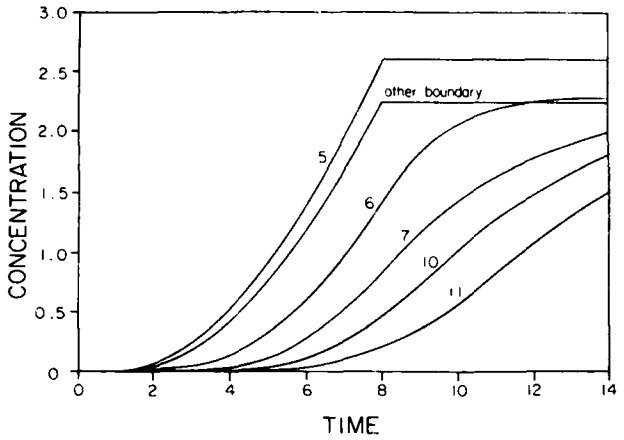

Fig. 4*a*. A biased calculation in which box 5 had the (by definition erroneous) concentration shown, leading to the erroneous final state shown in Figure 4*b*.

sought. Then there exists an adjoint system trajectory $\lambda(t)$ such that

$$\lambda(t) = \mathbf{A}^T\lambda(t+1) \tag{8}$$

subject to the adjoint terminal boundary condition

$$\lambda(t_f) = 2\mathbf{G}(\mathbf{C}(t_f) - \mathbf{C}_d) \tag{9}$$

and such that the Hamiltonian (7) is stationary over $\mathbf{u}$:

$$\frac{\partial H}{\partial \mathbf{u}} = 0 \tag{10}$$

(This theorem has direct generalizations to nonlinear systems and continuous time ones.)

Applying the theorem to the system (4), the Hamiltonian minimum condition leads to

$$\mathbf{B}^T\lambda(t) = -2\mathbf{u}(t) \quad \mathbf{u}(t) = -(1/2)\mathbf{B}^T\lambda(t) \tag{11}$$

giving the control in terms of λ. The λ are Lagrange multipliers, and perhaps the most important thing we can observe about them is that they satisfy an evolution equation (8), involving backwards running time, and the adjoint of the matrix $\mathbf{A}$. Such adjoint systems pervade control problems and have been widely recognized [e.g., *Lewis and Derber*, 1985; *LeDimet and Talagrand*, 1986; *Thacker and Long*, 1988] as the key to system sensitivity. In the present case, the λ represent the systematic, stable, backwards propagation of information about the terminal constraint to the prior time history of the system. It can be shown that the Green's functions employed in P2 satisfy the adjoint system (8). As is usually the case [e.g., *Schröter and Wunsch*, 1986], the λ are readily interpretable as the sensitivity of the objective function to perturbations in the tracer concentration $\mathbf{C}(t)$ at any time t, i.e.,

$$\Delta J(t) = -\lambda^T(t)\Delta\mathbf{C}(t) \tag{12}$$

To solve this system (equations (7)–(9)) and (11), we must find $\lambda(t)$ and $\mathbf{C}(t)$ such that (7) and (9) are simultaneously satisfied. The system is awkward because the $\mathbf{C}(t)$ evolution equation must be solved forwards in time, and the $\lambda(t)$ equation backwards in time, with the boundary conditions on $\mathbf{C}$ applied at $t = 0$, and those for λ at $t = t_f$. This latter condition is particularly awkward because the value of $\mathbf{C}(t_f)$ appearing in (9) is unknown until the problem is solved.

Proceeding with $\mathbf{A}$ constant, it follows from (8) that

$$\lambda(t) = (\mathbf{A}^T)^{t_f - t}\lambda(t_f) \tag{13}$$

and specifically that

$$\lambda(0) = (\mathbf{A}^T)^{t_f}\lambda(t_f) = (\mathbf{A}^T)^{t_f}2\mathbf{G}[\mathbf{C}(t_f) - \mathbf{C}_d] \tag{14}$$

We can therefore develop the following sequence from (4):

$$\mathbf{C}(1) = \mathbf{A}\mathbf{C}_0 - \mathbf{B}\mathbf{B}^T\lambda(0)/2 = \mathbf{A}\mathbf{C}_0 - \mathbf{B}\mathbf{B}^T(\mathbf{A}^T)^{t_f}\mathbf{G}(\mathbf{C}(t_f) - \mathbf{C}_d)$$

$$\mathbf{C}(2) = \mathbf{A}\mathbf{C}^{(1)} - \mathbf{B}\mathbf{B}^T\lambda(1)/2 = \mathbf{A}^2\mathbf{C}_0 - \mathbf{A}\mathbf{B}\mathbf{B}^T\lambda(0)/2 - \mathbf{B}\mathbf{B}^T\lambda(1)/2$$

$$= \mathbf{A}^2\mathbf{C}_0 - \mathbf{A}\mathbf{B}\mathbf{B}^T(\mathbf{A}^T)^{t_f}\mathbf{G}(\mathbf{C}(t_f) - \mathbf{C}_d) - \mathbf{B}\mathbf{B}^T(\mathbf{A}^T)^{t_f - 1}\mathbf{G}(\mathbf{C}(t_f) - \mathbf{C}_d)$$

$$\vdots$$

$$\mathbf{C}(t_f) = \mathbf{A}\mathbf{C}(t_f - 1) - \mathbf{B}\mathbf{B}^T\lambda(t_f - 1)/2$$

$$= \mathbf{A}^{t_f}\mathbf{C}_0 - (\mathbf{A})^{t_f - 1}\mathbf{B}\mathbf{B}^T(\mathbf{A}^T)^{t_f}\mathbf{G}(\mathbf{C}(t_f) - \mathbf{C}_d) + \cdots \tag{15}$$

Using (13) and (14) we see that this last expression involves only terms in $\mathbf{C}(t_f)$, $\mathbf{C}_0$, and $\mathbf{C}_d$ on the right. Collecting all the coefficients of $\mathbf{C}(t_f)$ on the left-hand side, we can solve explicitly for $\mathbf{C}(t_f)$ by a single matrix inversion. (The matrix dimension is that of $\mathbf{A}$. Existence of the inverse of this matrix

1	2 2.252	3 2.252	4
5 3.552	6 2.618	7 2.093	8 0
9 2.252	10 2.003	11 1.600	12 0
13	14 0	15 0	16

Fig. 4*b*. Concentration resulting at t_f when flow is precisely the same as in Figures 1 and 3. For obvious reasons, the "right" model leads to an erroneous terminal state.

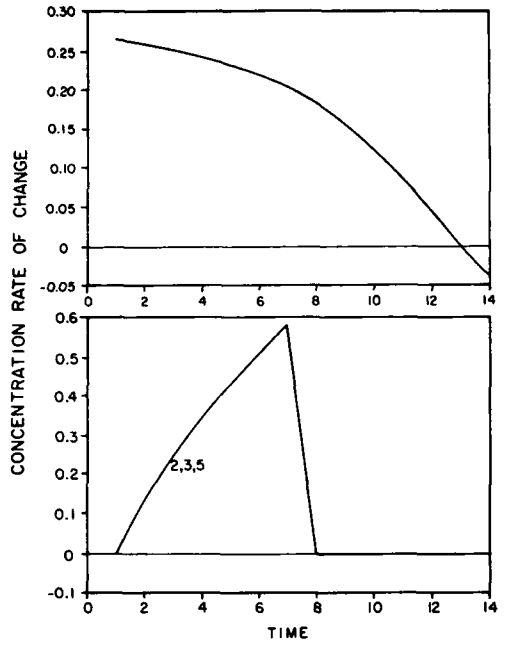

Fig. 5*a*. Bottom panel shows concentration rates of change **u** in boundary boxes 2, 3, and 5 (same as the time histories displayed in Figure 3). Top panel displays the concentration rates of change as determined from control solutions of (15), (8), and (11). These differ markedly from the "correct" solution in the lower panel, but drive the model to the observed terminal concentrations, within slight permissible errors. The top panel histories are those with smallest mean square with that property and clearly demonstrate the nonunique character of the terminal constraint solution. Box 9 is a passive reservoir, and hence the value of **Bu** there is set to zero.

is related to the ideas of "controllability" and "observability" of a system, which we will not take up here. Should the matrix be singular, various generalized inverses can be used.)

With $\mathbf{C}(t_f)$ then known in terms of $\mathbf{C}_0$ and $\mathbf{C}_d$, we can now go back and calculate **u** explicitly, as well as $\mathbf{C}(t)$. The control **u** is what is known as an "open-loop" one, because it involves only $\mathbf{C}(t = 0)$ and $\mathbf{C}_d(t_f)$, both of which are external parameters. (So-called closed-loop, or feedback controls, with $\mathbf{u}(t) \propto \mathbf{C}(t)$ can be obtained from this solution.) For one example, we took $\mathbf{G} = \mathbf{I}$ and $\mathbf{C}_d(t_f)$ from Figure 3*b*. The simple form of **B** shown in Figure 2 was retained. The solution that resulted gave a control variable **u** as depicted in Figure 5*a* and an interior time history as shown in Figure 5*b*. The terminal state (Figure 5*c*) found differs slightly from the "true" terminal state of Figure 3*b* because we permitted a tradeoff between deviations from the exact observations and minimization of **u** over the time history. When $\mathbf{G} = 10\mathbf{I}$, the terminal state resulting (not shown) is closer to the observations, but the magnitude of **u** has necessarily increased. The λ are displayed in Figure 5*d*.

These solutions were obtained in a two-pass system: we have to solve the system once completely to determine $\mathbf{C}(t_f)$ and then again to calculate $\mathbf{C}(t)$. But if the control **u** is acceptable, we have demonstrated that our model has passed its consistency requirements for reproducing the terminal state. If no acceptable **u** can be found, then we are assured that no error in the boundary conditions can explain the failure, and we must modify the **A** matrix (i.e., the J_{ij} parameters defining this model). In carrying out the calculations just described, a lot of matrix multiplications, but only one matrix inversion, of a matrix of dimension equal to the number of boxed, are required.

2.4. *Further Constraints*

A not uncommon tracer situation is one in which two or more surveys are available and the boundary conditions and other information must be consistent with both. (A restricted version of this situation was solved in P2).

A second form of constraints on the boundary conditions are represented in the problem worked, through supposed knowledge of the surface boundary concentration histories; i.e., we did not use directly any knowledge of $\mathbf{C}(t)$ in the surface boxes. This type of information can be accommodated in a number of ways [e.g., *Stengel*, 1986]. One simple approach is to modify the objective function from (5) to

$$J = [\mathbf{C}(t_f) - \mathbf{C}_d]^T \mathbf{G} [\mathbf{C}(t_f) - \mathbf{C}_d] + \sum_t [\mathbf{u}(t) - \mathbf{u}_0(t)]^T \mathbf{F} [\mathbf{u}(t) - \mathbf{u}_0(t)]$$

where $\mathbf{u}_0$ represents any prior estimate of what the control ought to be and **F** is another reciprocal covariance matrix. The calculation proceeds as before, with the second-term of the Hamiltonian in (7) modified appropriately.

2.5. *Time-Dependent Inversion*

Although we will not pursue it in detail at this time, the control formalism suggests an approach to model change if it must be modified to bring it into accord with the observations, simple changes in the boundary conditions having proved inadequate. We only sketch the procedure, leaving details to the future.

A standard control representation is the so-called feedback form:

$$\mathbf{u} = -\mathbf{K}(t)\mathbf{C}(t) \tag{16}$$

where the control at time t is chosen to depend explicitly upon the value of the state at that time. (The form used in section 2.3 is the so-called open loop control representation; text-

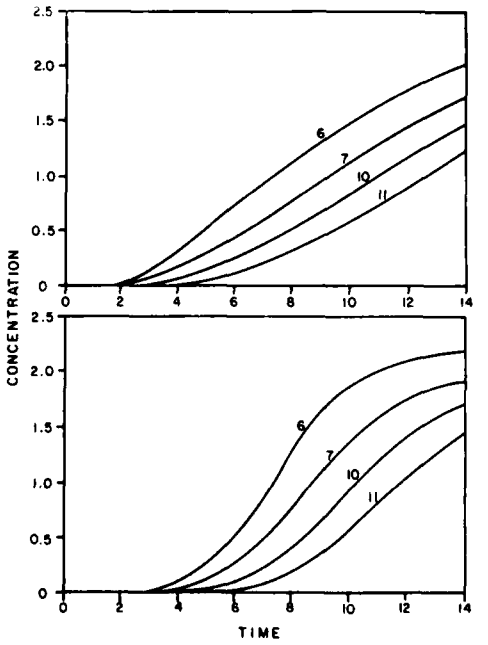

Fig. 5*b*. Bottom panel shows concentration time histories in the interior boxes in the reference calculation (same as depicted in Figure 3*a*), and the top panel interior time histories when driven by the boundary control of upper panel of Figure 5*a*.

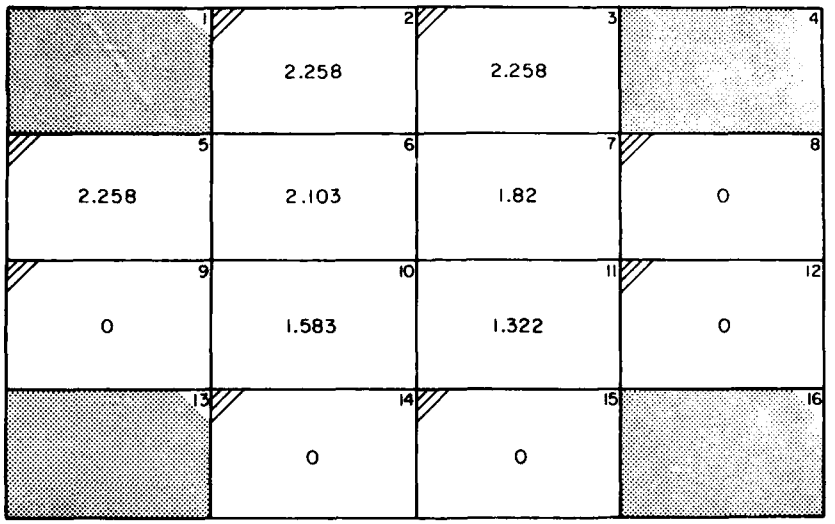

Fig. 5c. Terminal state corresponding to Figures 6a and 6b, and differing from the correct state of Figure 3b because $G = 1.0\mathbf{I}$ and the tradeoff permitted between deviation from the terminal constraint and the magnitude of $\mathbf{u}$.

books show how to derive one from the other.) As before, some objective function involving $\mathbf{u}$ is chosen to reflect the needs of the particular situation. Suppose the boundary conditions are held fixed, and the control is applied instead to the model parameters.

In feedback form, (4) becomes

$$\mathbf{C}(t+1) = \mathbf{A}\mathbf{C}(t) - \mathbf{B}\mathbf{K}(t)\mathbf{C}(t)$$

$$= (\mathbf{A} - \mathbf{B}\mathbf{K}(t))\mathbf{C}(t) = \mathbf{A}'(t)\mathbf{C}(t) \qquad (17)$$

absorbing $\mathbf{K}$ into $\mathbf{A}$ to generate a new system matrix $\mathbf{A}'$. If an appropriate $\mathbf{K}$ has been found which reproduces the required terminal constraint, one has a modified model, given by $\mathbf{A}'$, which is consistent with the observed data.

This latter conclusion can be accepted only if the structure of $\mathbf{A}'$ is physically consistent. Thus the elements of $\mathbf{A}$ are composed of balancing sums of the J_{ij} as discussed in section 2. To assure that $\mathbf{A}'$ has elements J_{ij}' satisfying mass conservation in each box would require solving the feedback control problem subject to these additional constraints. In principle, these additional constraints can be accommodated by existing control methods, but such a model modification procedure has not yet been attempted in practice for the tracer problem.

If $\mathbf{K}(t)$ is permitted to vary with time, the new J_{ij}' found would also be time-dependent. One can anticipate that feedback control methods will eventually provide the key to inverting models with time-dependent flow fields.

3. State Estimation

3.1. *Recursive Improvement, Forward in Time*

Control methods encompass a variety of goals associated with time evolving systems and their connection with realistic observations. Section 2 was directed to control per se, relating missing boundary conditions to observations of a terminal state. The calculation of the state $\mathbf{C}(t)$ given the set of observations (2) while simultaneously improving prior estimates of the boundary condition is also advantageously examined in the control format because it permits a flexible and efficient approach to combining data with observations.

Several reasons exist for tackling the state estimation problem, as distinct from the control problem just described. The nature of oceanographic observations is such that they are acquired over significant periods of time, often with large temporal gaps in any given area. One may have previously estimated the tracer distribution within the ocean up to and including the time t_1, of some prior survey. With new data available, one seeks to make a best estimate of the field using the new data, without having to recompute all the previous history as well. The fundamental motivation is that the observations obtained at $t_f > t_1$ carry information that ought to be useful in improving the estimate of the state at t_1 and earlier.

Suppose at time t we observe the tracer concentrations, in i boxes in the set I, $i \in I$. Define the square matrix $\mathbf{E}$ as having dimension equal to the total number of boxes, and let all its elements vanish except for unity along the diagonal in row or column i. Then the observations $\mathbf{z}(t)$ at time t can be written

$$\mathbf{z}(t) = \mathbf{E}\mathbf{C}(t) + \mathbf{n}(t) \qquad (18)$$

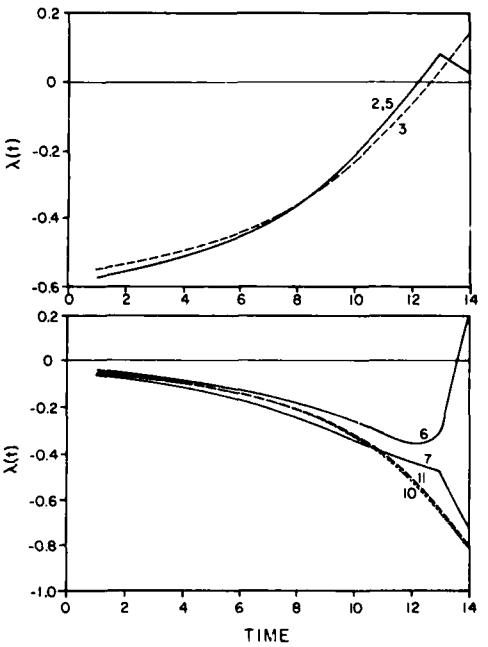

Fig. 5d. Adjoint solution (Lagrange multipliers) for problem displayed in Figures 5a–5c. Not surprisingly, the most important constraints are the evolution equations at times near the terminal time.

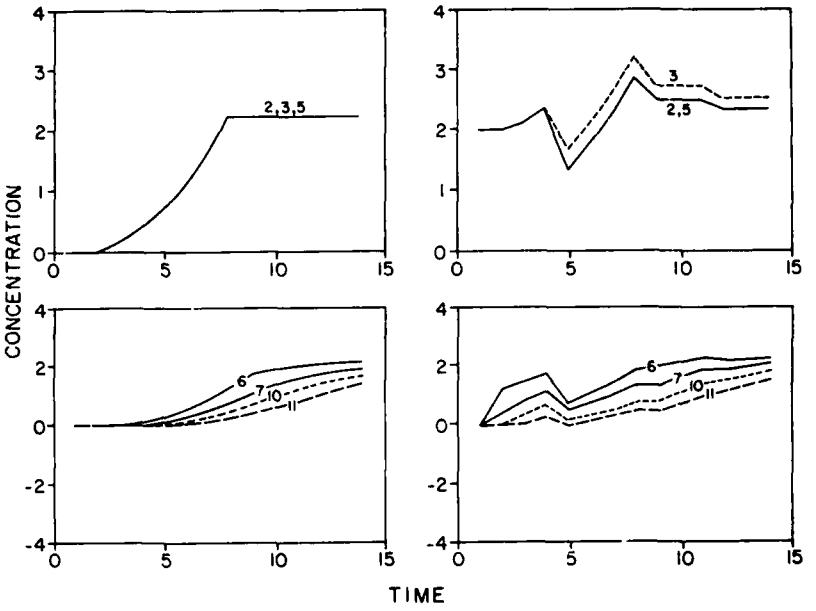

Fig. 6. (Left) Correct concentration values for boundary (top) and interior boxes (bottom). (Right) Kalman filter estimate, with observations of the interior made available at times 5, 9, and 12. Initial boundary concentrations were set to a value of 2, (correct value is 0); initial interior concentrations were set to 0, but with a large error estimate. Note convergence to correct values as more data are acquired.

where $\mathbf{n}$ represents the observational noise whose mean is assumed 0 and whose covariance is $\mathbf{R} = \langle \mathbf{n}\mathbf{n}^T \rangle$.

Suppose that an estimate of $\mathbf{C}$, called $\hat{\mathbf{C}}(0)$, is known at some *initial time* $t = 0$ *(it might be zero) and with an error* covariance

$$\mathbf{P}(0) = \langle (\hat{\mathbf{C}}(0) - \mathbf{C}(0))(\hat{\mathbf{C}}(0) - \mathbf{C}(0))^T \rangle$$

An estimate $\hat{\mathbf{C}}(1)$ of $\mathbf{C}$ one time step in the future is computable from (4) and is

$$\hat{\mathbf{C}}(1, -) = \mathbf{A}\hat{\mathbf{C}}(0) + \mathbf{B}\mathbf{u}(0) \tag{19}$$

(the reason for the minus sign will become clear). If the initial state estimate is uncertain, then surely the calculation (19) is also uncertain. It can be shown without difficulty [*Brogan*, 1982] that the uncertainty of $\hat{\mathbf{C}}(1, -)$ is

$$\mathbf{P}(1, -) = \mathbf{A}\mathbf{P}(0)\mathbf{A}^T + \mathbf{Q} \tag{20}$$

$\mathbf{Q}$ has been introduced to represent the covariance of any unobservable or unpredictable contribution to the driving term in (4) This noise process is assumed to have zero mean.

If some observations $\mathbf{z}(1)$ become available at $t = 1$, they will in general differ from the initial estimate (19). If the difference between estimate and observation lies outside the estimated uncertainty of both $\mathbf{z}(1)$, $\mathbf{C}(1)$, it seems reasonable that we should be able to combine the measurement with the initial estimate, with due regard for the relative errors of both, into a better estimate of $\mathbf{C}(1)$ than is represented by either alone. We therefore demand an improved estimate, following the initial calculation (19) and the observation in the form

$$\hat{\mathbf{C}}(1, +) = \hat{\mathbf{C}}(1, -) + \mathbf{K}[\mathbf{z}(1) - \mathbf{E}\hat{\mathbf{C}}(1, -)] \tag{21}$$

where the "gain matrix" $\mathbf{K}$ must be determined. Structurally, the logic is simple. In the absence of any observation, the best estimate we can make should reduce to the calculated one, i.e., $\mathbf{K} = 0$; if the difference between observation and calculation is large, and if, for example, the observational noise is much less than the uncertainty expressed in (20), then $\mathbf{K}$ becomes the generalized inverse of $\mathbf{E}$; i.e., the observations replace the calculations. Thus the minus sign in the argument denotes an estimate made from the evolution equation alone, and the plus sign the modified estimate made after the observations are used.

A general expression for $\mathbf{K}$ can be derived that minimizes the mean square error of the estimate. It is [e.g., *Liebelt*, 1967]

$$\mathbf{K} = \mathbf{P}(1, -)\mathbf{E}^T(0)[\mathbf{E}(0)\mathbf{P}(1, -)\mathbf{E}^T(0) + \mathbf{R}]^{-1} \tag{22}$$

(The behavior we anticipated $\mathbf{K}$ would have can be confirmed by examination of this expression). The expected error of this new estimate (21) can be shown to be

$$\mathbf{P}(1, +) = [\mathbf{P}(1, -)^{-1} + \mathbf{E}^T(0)\mathbf{R}^{-1}\mathbf{E}(0)]^{-1}$$
$$= \mathbf{P}(1, -) - \mathbf{K}\mathbf{E}\mathbf{P}(1, -) \tag{23}$$

Readers may recognize the forms (20)–(23) as a Kalman filter operation. M. Ghil [e.g., *Ghil et al.*, 1981] has pioneered this approach to meteorological updating and forecasting and a small oceanographic literature has followed that path [e.g., *Brammer et al.*, 1983; *Miller*, 1986]. The new estimate (19) then replaces $\hat{\mathbf{C}}(0)$ and time evolves, leading to the recursion

$$\hat{\mathbf{C}}(t + 1, -) = \mathbf{A}\hat{\mathbf{C}}(t, +) + \mathbf{B}\mathbf{u}(t) \tag{24a}$$

$$\mathbf{P}(t + 1, -) = \mathbf{A}\mathbf{P}(t, +)\mathbf{A}^T + \mathbf{Q} \tag{24b}$$

$$\mathbf{K}(t) = \mathbf{P}(t + 1, -)\mathbf{E}^T(t) \cdot [\mathbf{E}(t)\mathbf{P}(t + 1, -)\mathbf{E}(t)^T + \mathbf{R}(t)]^{-1} \tag{24c}$$

$$\mathbf{P}(t + 1, +) = [\mathbf{P}(t + 1, -)^{-1} + \mathbf{E}(t)^T\mathbf{R}^{-1}(t)\mathbf{E}(t)]^{-1}$$
$$= \mathbf{P}(t + 1, -) - \mathbf{K}(t)\mathbf{E}(t)\mathbf{P}(t + 1, -) \tag{24d}$$

$$\hat{\mathbf{C}}(t + 1, +) = \hat{\mathbf{C}}(t + 1, -) - \mathbf{K}[\mathbf{z}(t + 1) - \mathbf{E}\hat{\mathbf{C}}(t + 1, -)] \tag{24e}$$

At time steps with no observations, $\mathbf{K}$ vanishes, and we simply continue without it.

Figure 6 shows how such a calculation could work in prac-

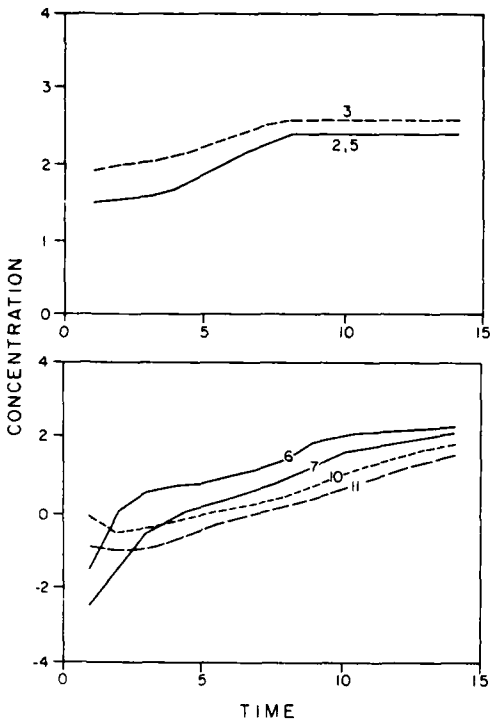

Fig. 7. Smoothed boundary (top) and interior (bottom) values. Compare to Figure 6.

tice. The initial concentrations in the boundary boxes were (deliberately erroneously) set to $\mathbf{C} = 2$ (the correct value being zero). The initial interior concentrations were correctly set to zero. Figure 6(left) compares the correct interior concentrations through time with those calculated using the initially incorect boundary data. For the first four time steps, the interior estimates diverge rapidly from the correct values because the erroneously high boundary estimates rapidly dye the interior boxes.

At time $t = 5$, observations are introduced in the interior boxes only, with an estimated error covariance of $\mathbf{R} = 1.0\mathbf{I}$. This set of noisy observations drives the estimated interior observations toward the correct values. Another set of observations is introduced at time step 9, and again at time step 12. As more observations are included the system state estimate is gradually converging toward the correct values.

For purposes of this illustration, the error in all the initial boundary concentrations was taken to have a variance of 5, in boxes = 2, 3, and 5 and $\mathbf{Q} = 0.1\mathbf{I}$. In this instance, $\mathbf{Q}$ represents the error owing to the failure to specify the values of $\mathbf{Bu}$.

Even though the assumption was made that no subsequent boundary concentration observations were available following the initial estimate, Figure 6 shows that the interior observations are able to improve the estimates of the boundary concentrations too, simply because boundary values and interior observations are connected through the system evolution matrix $\mathbf{A}$.

(All estimates shown are accompanied by a complete error covariance matrix which has not been displayed to keep the figures uncluttered.)

3.2. *Smoothing*

Meteorological oceanographic practice until recently has focussed on the forecasting calculation, represented by (24*a*). We now part company with that emphasis by noting the evolving and accumulating observations carry information about the tracer concentrations prior to the time of observation. How can an observation of $\mathbf{C}(t_f)$ be used to help improve an estimate of $\mathbf{C}(t)$, where $t < t_f$? (We previously employed $\mathbf{C}(t_f)$ to help estimate $\mathbf{u}$ at prior times; the present problem seeks instead to use the available information to estimate $\mathbf{C}(t)$ both on boundaries and in the interior.) The question leads to the Kalman "smoother"; we follow *Liebelt* [1967, p. 198] and *Meditch* [1973] and use the *Rauch et al.* [1965] algorithm. Recent meteorological work [e.g., *LeDimet and Talagrand*, 1986] directed at improving estimates of the initial state of the atmosphere from subsequent observations are a similar application of the smoothing method.

Derivation of the algorithm is lengthy (more so than for the Kalman filter) and is not described here. We suppose that we have retained all prior estimates $\hat{\mathbf{C}}$ and $\mathbf{P}$ from the forward in time calculation (22). Then using the plus sign to denote the improved estimate, the Kalman smoothing calculation is

$$\hat{\mathbf{C}}^+(t) = \hat{\mathbf{C}}(t) + \mathbf{J}(t)(\hat{\mathbf{C}}^+(t+1) - \mathbf{A}\hat{\mathbf{C}}(t)) \tag{25a}$$

$$\mathbf{P}^+(t) = \mathbf{P}(t,+) + \mathbf{J}(\mathbf{P}^+(t+1) - \mathbf{P}(t+1,-))\mathbf{J}^T \tag{25b}$$

$$\mathbf{J}(t) = \mathbf{P}(t,+)\mathbf{A}^T\mathbf{P}(t+1,-)^{-1} \tag{25c}$$

$$\mathbf{P}(t+1,-) = \mathbf{A}\mathbf{P}(t,+)\mathbf{A}^T + \mathbf{Q} \tag{25d}$$

($\mathbf{J}$ should not be confused with the objective function J or the flow parameters J_{ij}). Notice particularly the appearance of the transpose of $\mathbf{A}$ in (25*c*), which should be no surprise in view of its previous appearance as the fundamental quantity for carrying information backwards in time. The essence of the calculations is a comparison of the prior estimate of $\mathbf{C}(t)$ with the value computed backwards from later observations and a modification to the prior estimate as an appropriately weighted average of the two values. The observations themselves do not appear in (25) because the information they carry has already been extracted in making the Kalman filter estimate.

All information has now been exhausted. There is nothing further to be gained by another calculation in the forward direction: the estimates would not change unless more observations became available.

The Kalman smoother (25) was used to reestimate the values of $\mathbf{C}$. The result is shown in Figure 7. Notice the great improvement in the values at times when no observations were previously available, including the much improved estimate of the incorrect initial state. Comparison of the smoothed estimate in the interior shows that the backward propagation of the future observations has generally improved the estimates compared to those from the Kalman filter estimates. At early times prior to the first observations at $t = 5$, the smoothed interior estimates diverge from the true state, going unphysically negative. The apparent reason for this behavior was the use of a large initial error estimate, for the interior initialization at $t = 0$. When the initial interior error estimate was made much smaller, the system drove the estimates of the initial boundary concentrations much closer to zero, rather than permitting them to asymptote to nonzero values, and the interior initial values of 0 were much more closely recovered (this case is not shown here).

The error estimates for the interior values at $t = 0$ in Figure 7 are $\approx \pm 1.5$ and thus within the formal errors, are unphysical negative values are indistinguishable from zero. It is also clear that imposition of positivity constraints on the system would be helpful additional information.

4. SOME GENERAL COMMENTS

The Kalman filter has been much discussed and used since its introduction in 1960 (see the history in *Sorenson* [1985]). Although sometimes appearing extremely mysterious, the basic ideas it embodies are straightforward, and our own discussion here has not introduced anything original into the subject. The purpose of its discussion here is twofold: the application of the filter method into an advection-diffusion system does seem to have some practical result, and more important, the control ideas described above, and the Kalman state estimation are so-called dual problems of each other [see *Stengel*, 1986]. That is, somewhat surprisingly, the control problem and the state estimation problem, both of which rely upon a state estimate, are mathematically equivalent.

The numerical operations demanded by the algorithm discussed here are easy to implement for small-scale systems (all the examples displayed were generated on an IBM PC-XT using the software system entitled PC-MATLAB, for which matrix operations are both easy to code, and very fast). For basin scale general circulation models, the number of degrees of freedom grows rapidly to the point that mere storage of the arrays becomes a major problem. (In the alternative dynamic programming approach to control, the size issue is colorfully known by the mathematician Richard Bellman's label as "the curse of dimensionality".)

We paid almost no attention here to the question of the extent to which the implementation of equations such as (25) remains feasible for ocean basin models [*Ghil et al.*, 1981, *Thacker and Long* [1988] and others however discuss the question for equation (24) at considerable length). There are two distinct reasons for this neglect. First, it is useful to separate understanding of ideal solutions from questions of practical implementation. The intellectual demands of the methods described are sufficiently great that distractions of numerical efficiency are best delayed. Second, the rate of improvement both in computing power and numerical algorithms remains so rapid, that computations infeasible today may well become almost trivial in 10 years. Thus it seems unnecessary to be concerned overly much at this stage with detailed questions of precisely what size problems are feasible or not.

Nothing has been said here about direct use of the continuous time formulation of the control problem; we went immediately from (1) to (4). As with inverse methods, confusion has been engendered by claims that continuous time methods (variational principles) have some intrinsic advantage over discrete methods. To my knowledge, there are no practical problems in which one cannot formulate the problem wholly as a discrete one. There may be difficult questions of what constitutes an adequate discretization, but that problem is separable from the question of whether or not the fundamental practical questions can be answered, given that a sensible discretization has been carried out. There is little doubt that the continuous time formulations are mathematically elegant (lying largely in the realm of functional analysis) and interesting (see *Lions* [1971] and the collection of papers edited by *Stavroulakis* [1983]). But the intuitive advantage of working in finite dimensional vector spaces, and the consequent ability to reduce most problems to some form of least squares should not be minimized. *Lanczos* [1961] makes particularly clear the connection between the continuous and discrete problems. We can also point directly at the control literature itself, wherein many textbooks develop the continuous and discrete control and estimation problems in parallel, with experience suggesting no intrinsic advantage of one approach over the other.

APPENDIX

We justify the assertion made in the text that a finite difference formulation of the tracer problem can be put in the canonical form of (4). For example, if we discretize the Laplacian with α a scalar, u and v constant, and using upwind differencing following *Roache* [1976], we have a simple explicit scheme:

$$C_{ij}^{t+1} - C_{ij}^{t} + R(uC_{ij}^{t} - uC_{i-1,j}^{t}) + R(vC_{ij}^{t} - vC_{i,j-1}^{t}) - d\{C_{i+1,j}^{t} + C_{i-1,j}^{t} - 2C_{ij}^{t} + (C_{i,j+1}^{t} + C_{i,j-1}^{t} - 2C_{ij}^{t})\} = 0 \qquad \text{(A1)}$$

$$R = U\Delta t/\Delta x \qquad d = \alpha\Delta t/\Delta x^2$$

U being a velocity scale and the other variables are conventional. (A1) is, in turn, of the form of the homogeneous version of (4), the boundary data being added in an obvious way. An implicit scheme would require an extra matrix inversion to reduce to (4).

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